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The object of this research is to characterize the molecular structures, energetics, spectroscopic properties, and elementary chemical reactions of the oxygen ring molecules O_4 through O_{12} and related species including $(NH)_n$ and C_n. The approach used will exploit recent developments in ab initio molecular quantum mechanics.

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FINAL TECHNICAL REPORT

Air Force Office of Scientific Research
Grant AFOSR-88-0167

"Fundamental Studies of Carbon, NH, and Oxygen Rings and Other High Energy Density Molecular Systems"

I. Summary

The development of efficient and safe conventional (i.e., non-nuclear) propellants and/or fuels is a goal of obvious technological significance. A desirable quality of such a propellant is clearly a high ratio of energy release to mass. The present research rests on a simple, but previously (i.e., before our work beginning in 1987) unrecognized, analogy between oxygen and sulfur. Our AFOSR supported research of the past four years has shown that the proposed oxygen ring systems are sufficiently promising to warrant further consideration. In fact, several experimental groups are now attempting to prepare and characterize oxygen rings in the laboratory. Thus a major emphasis in future phases of the HEDM (high energy density molecules) theoretical research is to work closely with Air Force supported experimental efforts to this end. Our work has also encouraged other theoretical groups to extend our S $\rightarrow$ O analogy to P $\rightarrow$ N, with the recent work of Lee and Rice on tetrahedral N_4 being a particularly beautiful example.

The potential attractiveness of oxygen rings follows from a number of considerations, including:

(a)   Our theoretical studies to date show that the cyclic O_n systems are definitely high energy density materials. This may be seen in Figure 1, kindly provided to us by Dr. Harvey Michels based on our predicted energetics for O_8;

(b)   As cryogenic solid propellants, oxygen rings may plausibly be expected to form a metastable condensed phase by analogy with the valence isolectronic sulfur rings, which of course are very stable solids under normal conditions;

(c)   The way to use oxygen rings as a rocket fuel is obviously analogous to that for normal molecular oxygen, i.e., O_2. Furthermore, burning of O_n with molecular hydrogen yields water as the only new molecular product. The absence of hazardous products (as opposed to other possible HEDM materials) of combustion is a strong argument in favor of oxygen rings.

Let us summarize the qualitative arguments concerning the energy content of the metastable O_n rings. First one notes that the valence-isoelectronic cyclic S_8 contains *no* energy in this sense. Specifically, gaseous S_8 lies 12.2 kcal per mole of sulfur atoms below four gas phase diatomic S_2 molecules. Can one guess this result using the dissociation energy of S_2 ($D_o = 4.37$ eV $= 100.8$ kcal/mole) and some reasonably standard S-S single-bond dissociation energy, say 54 kcal/mole? The answer to this question is a qualified "yes". Using this simple model, one predicts S_8 to lie (54-50.4) = 3.6 kcal/mole below four S_2 molecules on a per atom basis. By increasing the S-S bond energy from the standard 54 kcal to 63 kcal, the known experimental energy difference (+97.7 kcal) for

$$S_8 \; (g) \;\; \rightarrow \;\; 4 \, S_2(g) \tag{1}$$

H$_2$/O$_8$ Vacuum Specific Impulse

Chamber Pressure = 1000 psia
Exit pressure = 14.7 psia

H$_2$ + O$_8$

H$_2$ + O$_2$

Vacuum Specific
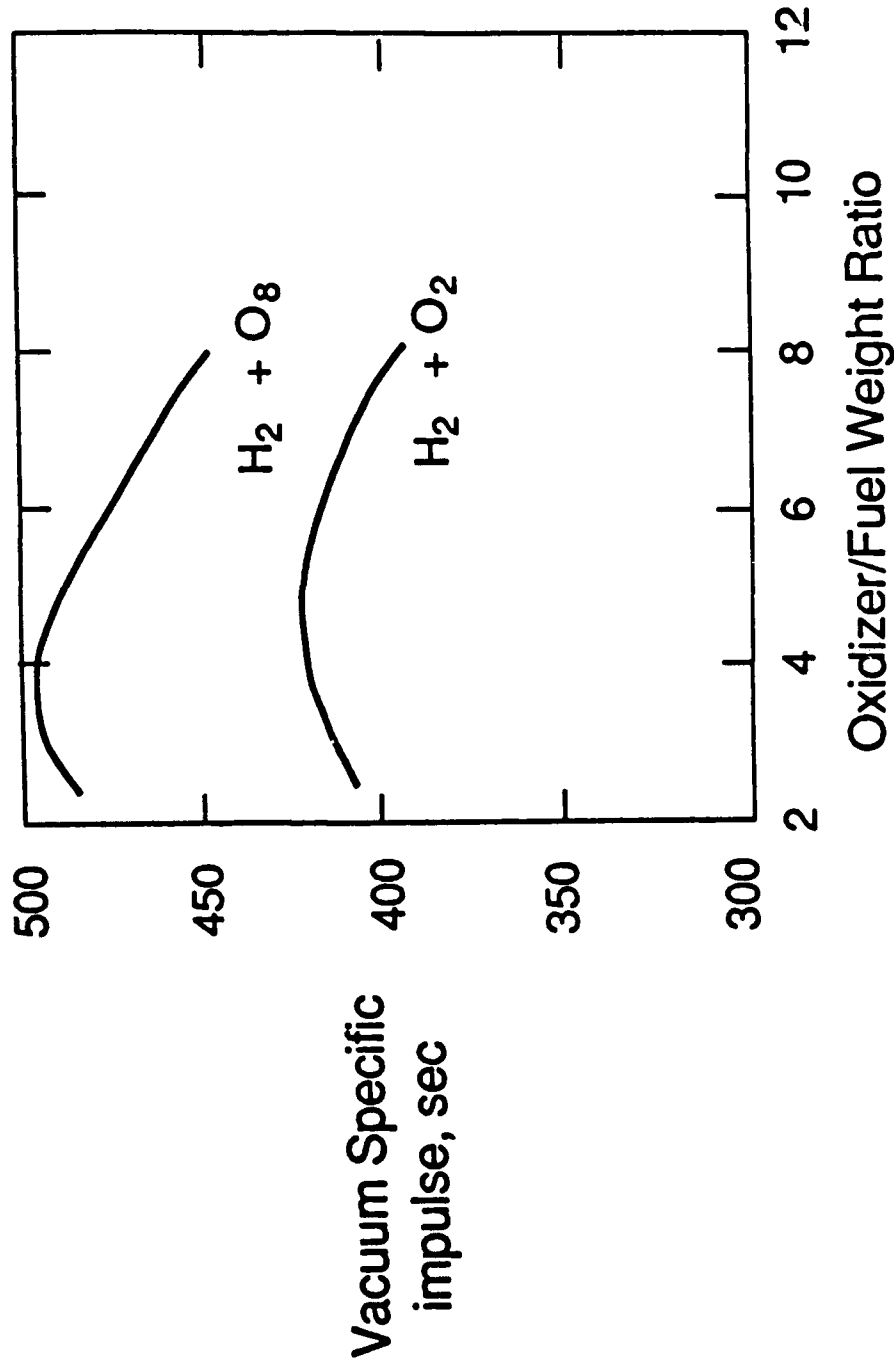impulse, sec

Oxidizer/Fuel Weight Ratio

Figure 1.   Specific impulse predictions for cyclic O$_8$.
Details are given in the text.

is precisely reproduced. This adjustment reflects the fact that the S-S bonds in S_8 are stronger than those in organosulfur compounds such as CH_3SSCH_3.

The comparable oxygen thermodynamic data make it immediately obvious why oxygen rings should be high energy density materials. First the standard O-O bond dissociation strength is 35 kcal/mole, *much weaker* than the 54 kcal for S-S bonds. Secondly, the dissociation energy of diatomic O_2 is D_o = 5.12 eV = 118.0 kcal/mole, *much stronger* than the 100.8 kcal for S_2. Thus the estimate for the energy stored in the "generic" oxygen ring is (35-59) = -24 kcal per mole of oxygen atoms. That is, the dissociation process

$$O_n \text{ (n even)} \;\rightarrow\; \frac{n}{2} O_2 \text{ (g)} \tag{2}$$
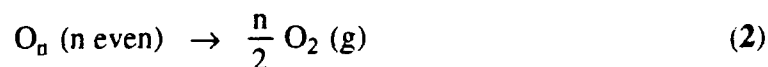
is estimated to be exothermic by 24 kcal per mole of oxygen atoms. Alternately, 48 kcal of energy is released per mole of O_2 molecules. A *larger* energy release is expected for the smaller rings, specifically O_4 and O_6, which presumably have smaller average O-O bond energies due to ring strain.

A principal accomplishment of the current AFOSR grant has been the prediction of the molecular structures and energetics of O_4, O_8, and O_{12}. References to our published work on these systems are given below. A careful, high level theoretical study of O_6 is currently underway. Figures 2 and 3 present our theoretical structures for O_8 and O_{12}. We are confident that these structures will be reliable should the oxygen rings prove susceptible to detailed molecular structure investigations in the laboratory.

What have we learned about the energetics of the oxygen rings? Let us first focus on the results for O_{12}. The valence isoelectronic sulfur molecule S_{12} at the DZ SCF level of theory is predicted to lie 21.9 kcal/mole below six S_2 molecules. This result may

1.400
1.414
1.358
1.438

105.6°
108.3°
108.4°
108.0°
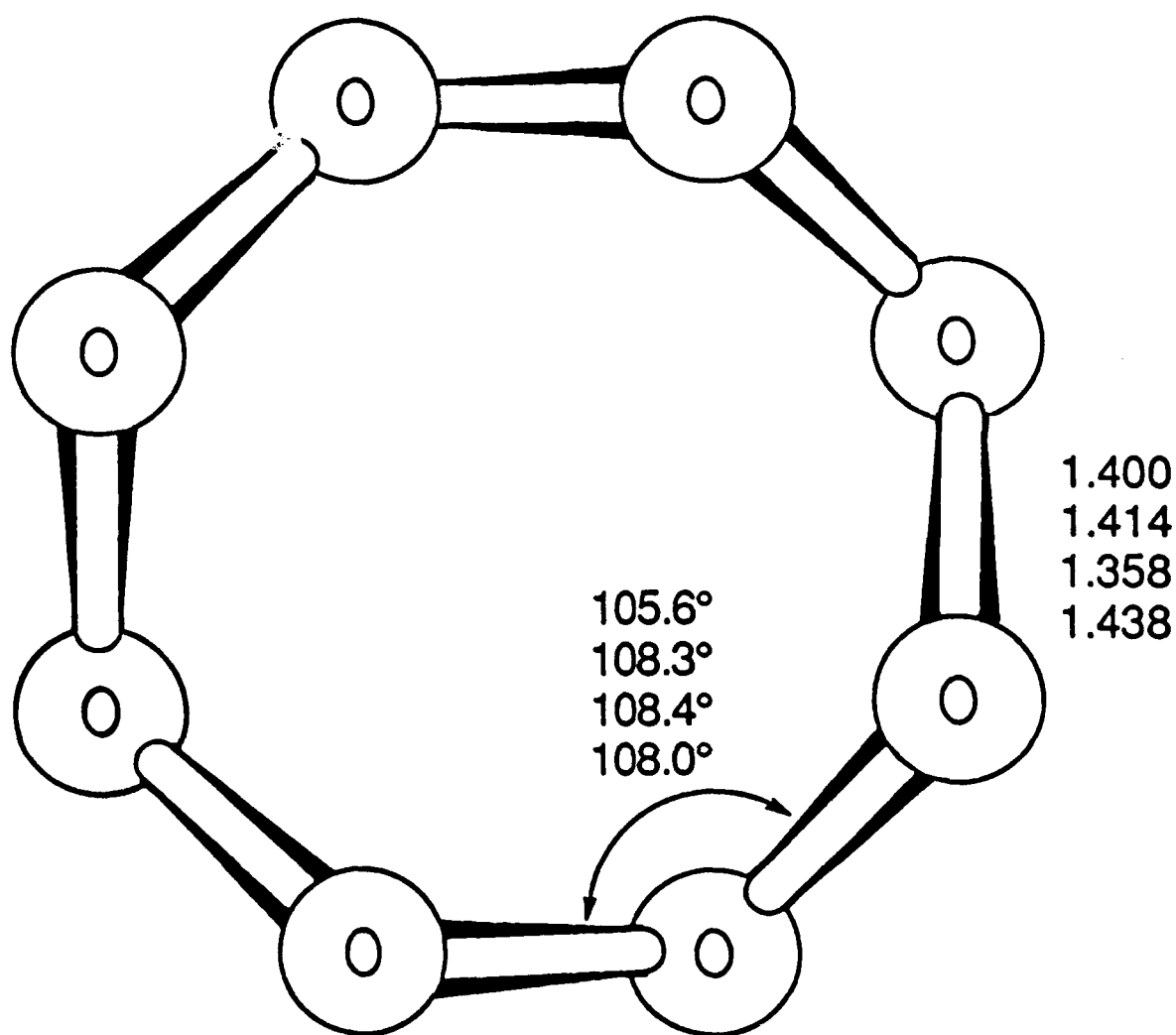
DIHEDRAL ANGLE =   101.5°   STO - 3G SCF
                     98.4°   DZ SCF
                     98.3°   DZ + P SCF
                     98.7°   DZ + P MP2

Figure 2. Predicted equilibrium geometries for cyclic O_8.
All bond distances are in Å.

Torsional $\theta(0000)$ = 88.0°
87.1°
86.9°
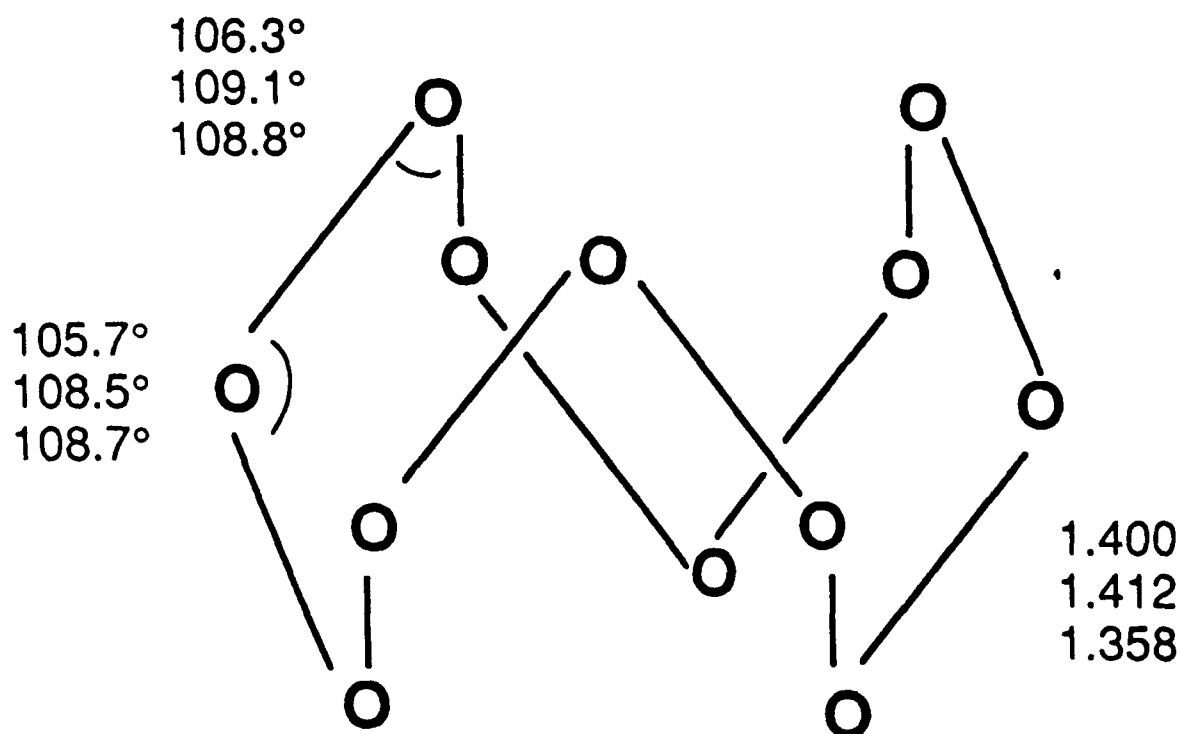
STO - 3G SCF

DZ SCF

DZ + P SCF

D_{3d} O_{12}

FIGURE 3.   Predicted self-consistent-field equilibrium
geometries for cyclic O_{12}. All bond distances
are in Å.

readily be translated into the prediction that S_{12} lies $21.9/12 = 1.8$ kcal/mole below separated S_2 molecules on a *per atom basis*. The analogous experimental value for gaseous S_8 is 12.2 kcal/mole per S atom. It is of course anticipated that DZ SCF theory will do a better job for 6 S_2 than for S_{12}, and an error of ~10 kcal/mole/atom seems to us to be perhaps less than might be expected. At the DZ SCF level O_{12} lies 20.9 kcal/mole *above* six O_2 molecules on a per atom basis. With the larger basis set DZ+P SCF method O_{12} lies 21.6 kcal/mole/atom above six separated diatomic oxygen molecules. Thus the addition of polarization functions (d functions on each oxygen atom) lowers the energy of 6 O_2 molecules somewhat more than that of O_{12}.

Analogous to S_{12}, one certainly expects that higher levels of theory (larger basis sets, and especially explicit treatment of electron correlation) will lower the energy of O_{12} relative to 6 O_2. Second-order perturbation theory supports this view. With the DZ basis set, the MP2 energy difference between O_{12} and 6 O_2 is 16.1 kcal/mole on a per O atom standard. These results suggest that O_{12} may be significantly more stable than our earlier back-of-the-envelope calculation (based on standard bond energies), which as discussed above indicated that generic cyclic O_n molecules might store 24 kcal per mole of oxygen atoms relative to the separated O_2 molecules.

Turning to the eight-membered rings, reported in Table I are the energies of O_8 and S_8 relative to the dissociation limits 4 O_2 and 4 S_2. Since experimental data is available for S, these results will be discussed first. At the DZ SCF and DZ+P SCF levels of theory, S_8 lies 13.0 and 33.9 kcal/mole, respectively, below four separated S_2 molecules. The latter (DZ+P SCF) result may readily be translated into the prediction that S_8 lies $33.9/8 = 4.2$ kcal/mole below separated S_2 molecules on a *per atom basis*. The analogous experimental value for gaseous S_8 is 12.2 kcal/mole per S atom.

Assuming the DZ+P SCF equilibrium geometry for S_8 (Figure 3), its dissociation energy has been predicted using second-order perturbation theory (MP2). However, for an open-shell system like the S_2 molecule $^3\Sigma_g^-$ ground state, the use of unrestricted Møller-Plesset second-order perturbation theory is most straightforward. At the S_2 RHF equilibrium geometry (DZ+P basis set, $r_e = 1.881$ Å) the UMP2 total energy is -795.25545 hartrees. The comparable MP2 energy for closed shell S_8 is -3181.11839 hartrees. Thus S_8 is predicted to lie 60.6 kcal/mole below 4 S_2 at this level of theory. On a *per atom* basis S_8 lies 7.6 kcal/mole below 4 S_2, in reasonable agreement with the experimental value 12.2 kcal/mole.

At the DZ SCF level O_8 lies 21.3 kcal/mole above four O_2 molecules on a per atom basis. With the larger DZ+P basis set O_8 lies 21.6 kcal/mole/atom above four separated diatomic oxygen *molecules* within the SCF approximation. Thus the addition of polarization functions (d functions on each oxygen atom) lowers the energy of 4 O_2 slightly more than that of O_8.

Assuming DZ+P SCF geometries, the DZ+P MP2 energies for O_2 and O_8 are -149.97388 and -599.68739 hartrees, respectively. Thus O_8 lies 130.6 kcal/mole above 4 O_2 or 16.3 kcal/mole higher on a per atom basis. Hence the effect of electron correlation is to significantly lower O_8 relative to the separated oxygen molecules.

More reliable yet should be the comparison of the energy of DZ+P MP2 geometry optimized O_8 with that of four comparable O_2 molecules. The O_2 geometry optimization is carried out at the DZ+P UMP2 level, yielding a bond distance $r_e = 1.253$ Å and total energy E = -149.97905 hartrees. Combined with the O_8 total energy, one predicts that cyclooctaoxygen lies 123.5 kcal/mole above four infinitely separated O_2 molecules. Thus geometry optimization is energetically much more important for O_8 with correlated methods than is the case for O_2. On a per atom basis the DZ+P MP2

Table 1. Total energies (in hartrees) for the cyclo-O_8 and cyclo-S_8 molecules at their fully optimized equilibrium geometries. Relative energies (ΔE) are given in kcal/mole.

	O_8	ΔE (O_8-$4O_2$)	S_8	ΔE (S_8-$4S_2$)
DZ SCF	-598.01365	+170.4	-3179.74094	-13.0
DZ+P SCF	-598.26838	+173.1	-3180.06123	-33.9
DZ+P MP2	-599.71940	+123.5	-3181.11839*	-60.6

*Energy evaluated at the DZ+P SCF equilibrium geometry.

dissociation energy for O_8 is 15.4 kcal/mole.

A number of significant relationships between the O_8 energetic predictions and those for O_{12} may be noted. First, the higher level theoretical methods used are broadly in agreement with the simpler methods used for O_{12}. For O_{12} the only correlated method used was DZ MP2 (using DZ SCF geometries) and those results were presented with great caution. However, the analogous DZ MP2 and DZ+P MP2 dissociation energies for O_8 are 15.7 and 16.3 kcal/mole/atom, respectively. The close agreement between the two methods suggests that our final O_{12} energetic predictions may be much more reliable than could reasonably have been anticipated.

Secondly the dissociation energies of O_8 and O_{12} appear to be very similar on a per atom basis. This may be seen from the following array of dissociation energies:

	O_8	O_{12}
DZ SCF	21.3	20.9
DZ+P SCF	21.6	21.6
DZ MP2	15.7	16.1

Both O_8 and O_{12} should be relatively free of bond angle and dihedral angle strain and their comparable energetics mirror those presumed for S_8 and S_{12} based on the latter's stability (the precise thermochemistry of gaseous S_{12} does not appear to be established). Thus one expects O_8 and O_{12} to be perhaps the most readily synthesizable of the oxygen rings.

Among the oxygen rings, the energetics have been most reliably established for what is apparently the least stable system, namely cyclotetraoxygen (Figure 4). Thus we are now able to make a reliable prediction of the heat of formation of cyclic O_4.

Using DZ+P CCSD energies, we can estimate the enthalpy change for converting four moles of O_3 to three moles of O_4. The electronic contribution to this enthalpy

1.392Å
1.433Å
1.473Å
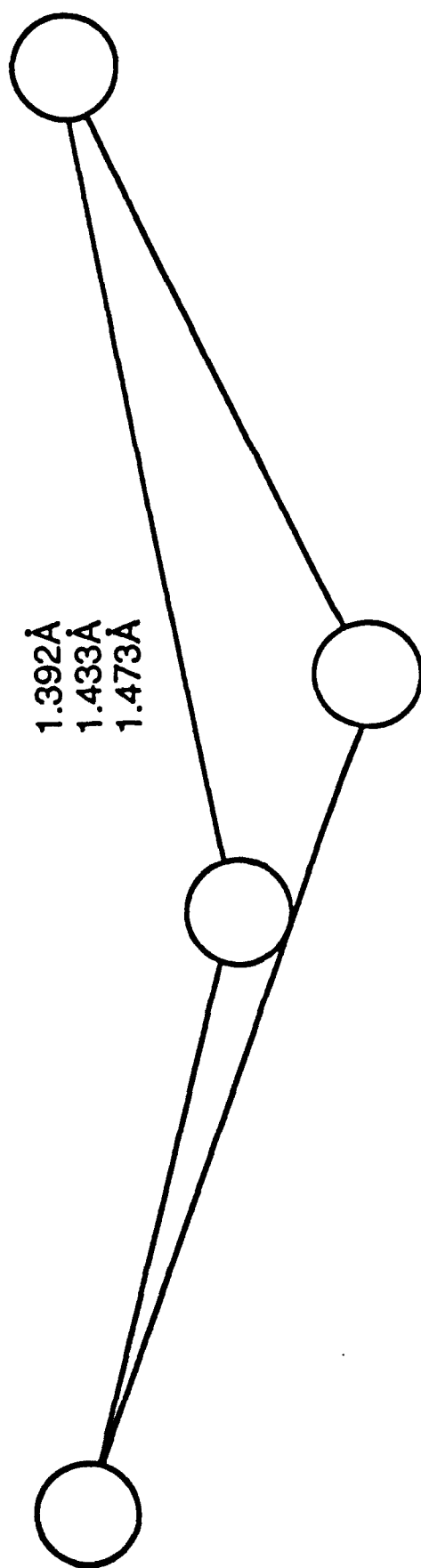
TORSIONAL ANGLE = 20.4° DZP SCF
24.8° DZP CISD
27.0° DZP CCSD

Figure 4.   Predicted equilibrium geometries for
cyclic O_4 at three distinct levels of theory.

change is 112.6 kcal/3 moles. The rotational and vibrational contributions to this enthalpy change total -1.5 kcal/3 moles. The experimental enthalpy of formation for O_3 is 34.1 kcal/mole or 136.4 kcal/4 moles. The enthalpy of formation of O_4 can be estimated by adding the enthalpy of formation for four moles of O_3 to the enthalpy change for converting four moles O_3 to three moles O_4. The enthalpy of formation of O_4 is therefore approximately 247.5 kcal/3 moles or 82.5 kcal/mole. The latter prediction is 17.5 kcal/mole lower than our previous estimate based on the DZ+P CISD level of theory. Some of the difference comes from the use of the experimental heat of formation for ozone. If this had been done for the CISD estimate, the result would have been 94.3 kcal/mol. Because of the size consistency of the CCSD method, the CCSD estimate is deemed to be more accurate than CISD. Thus the energetics of the O_4 system at equilibrium seem to be quite reliably established.

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IV. Relation to Work at Hanscom Air Force Base

On Monday, May 15, 1989 the Principal Investigator visited Hanscom Air Force Base with Dr. Larry P. Davis. After presenting a seminar describing our AFOSR-supported research, I spent the afternoon touring the laboratories of Drs. William A. M. Blumberg, Daniel H. Katayama, Edmond Murad, and John F. Paulson. During the accompanying discussions, several areas of mutual interest were developed. Dr. Davis later sent me written requests from the Hanscom research groups for specific collaborative studies. We have now completed work at Georgia on several of these projects. Our original AFOSR proposal included such visits to Air Force laboratories and collaborative efforts.

On Monday, April 23, 1990 the Principal Investigator visited Hanscom Air Force Base with Dr. Larry P. Davis. Following a seminar describing our recent AFOSR-supported research, I spent the afternoon with members of the research groups of Drs. Blumberg, Katayama, Murad, and Paulson. During these discussions, several additional areas of potential collaboration were brought to light. Dr. Davis later sent me written requests from the Hanscom research groups for joint efforts.